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Energy structure of high-temperature superconductors with the intersite Coulomb interaction

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Abstract. The effect of the intersite Coulomb interaction of fermions on the ground state and energy structure of high-temperature superconductors is considered within the three-band Emery model using an extended basis of the irreducible operators orthogonal on Mori. The proposed theory allows prediction of bands of the fluctuation states whose spectral intensity grows with an increase in the root-mean-square fluctuations of the occupation numbers. The increase in these fluctuations in high-temperature superconductors upon doping plays a key role in redistribution of the integrated density of the Fermi states.

PACS. 71.27.+a Strongly correlated electron systems; heavy fermions – 74.72.-h Cuprate superconductors – 71.28.+d Narrow-band systems; intermediate-valence solids

1 Introduction

Though the high-temperature superconductors (HTSC) were discovered long ago [1] the study of their electronic structure is one of the key directions in condensed matter physics. The description of the HTSC electronic properties is known to be nontrivial, which is caused by the presence of strong intra-atomic correlations. For instance, it requires careful consideration of these correlations to describe the ground state of copper oxides following the scenario for a Mott-Hubbard insulator [2].

An approach currently used for theoretical study of the electronic properties of ensemble of strongly correlated electrons is based on the known compromise, when a real system is simulated by the simplified model. On the one hand this model allows performing correct mathematical calculations and on the other hand keeps the most significant interactions of a real system under study. A classical example of this compromise is the Hubbard model [3]. In the first theoretical works dealing with HTSC this model was used to describe a non-phonon formation mechanism of the superconducting phase formation [4–6]. However, being one-band the Hubbard model cannot help to interpret experimental data on the electronic structure of copper oxides. In particular, the attempts to use this model for the description of angular resolved photoemission spectroscopy (ARPES) spectra taken from HTSC appear unsuccessful.

A model more convenient for the description of the HTSC electronic structure is the Emery model [7,8], which takes into account the electronic states of copper and oxy-

gen ions in an unit cell. In HTSC according to their chemical composition there are one copper ion and two oxygen ions per unit cell of the CuO_2 plane (Fig. 1). Therefore, even at the simplest consideration the energy spectrum of the Emery model is three-band, which complicates analytical calculations. In this context investigations concerning the possibility of obtaining the effective Hubbard-like Hamiltonians by means the cluster perturbation theory have been carried out [9–18]. Such an approach takes into account the strong intra-atomic interactions, but the correct description of the intersite Coulomb interaction between fermions located on copper and oxygen ions is problematical. In particular, as has been mentioned in [19] it is difficult to calculate the exchange integral within the cluster approach when the intersite interaction of holes on copper and oxygen ions is included into consideration. Consideration of only a CuO_4 cluster does not give correct results, since the effects of the interatomic Coulomb interaction depends on configurations of holes out of such a cluster. The situation is similar in the case when the energy band structure of the Emery model is calculated with account for the intersite correlations. Interest in the effects of the intersite correlations has quickened in the past few years, since was founded that an intersite charge fluctuations capable to induce the Cooper pairing of the fermions [20].

In view of the aforesaid, there is practical need in the development of a method for calculation of the Emery model energy structure that would make it possible to describe correctly not only the one-site interactions, but also the interactions of fermions located on different sites. This program may be realized by means of using an extended
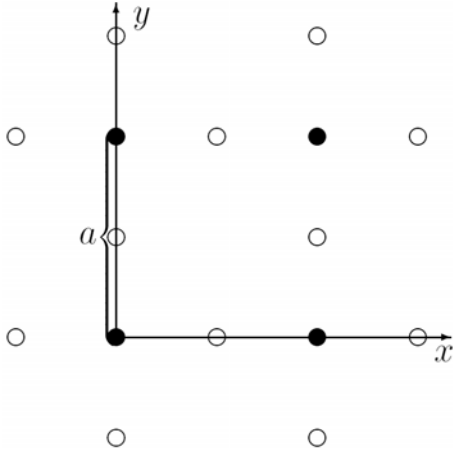
a e-mail: vvv@iph.krasn.ru

Fig. 1. CuO$_2$ plane of high-temperature superconductor.

basis of the irreducible operators orthogonal on Mori. In this work, we report the results of calculations of the energy band structure which have been obtained using the developed method.

2 Emery model in the strongly correlated regime

Let us consider a lattice of the HTSC CuO$_2$ plane, shown in Figure 1, where • – are Cu ions, ∘ – are O ions, a denotes a lattice constant, $\mathbf{x} = (a, 0)$ and $\mathbf{y} = (0, a)$ are lattice basis vectors. Each of the Cu ions has four adjacent O ions, and each of the O ions has two adjacent Cu ions. Without doping copper ions are in the divalent state Cu^{2+} ($3d^9$ state) corresponds to unfinished d shell. At the same time the oxygen ions O^{2-} is in the electronic configuration $2p^6$ corresponds to filled p shell.

The Emery Hamiltonian [7,8] describing the dynamics of electrons in CuO$_2$ planes of HTSC in the second quantized operators is given by

$$\hat{H} = \hat{H}_0 + \hat{T}_{pd} + \hat{T}_{pp}, \tag{1}$$

where

$$\hat{H}_0 = \varepsilon_d^0 \sum_{f\sigma} \hat{n}_{f\sigma}^d + U_d \sum_f \hat{n}_{f\uparrow}^d \hat{n}_{f\downarrow}^d + \frac{\varepsilon_p^0}{2} \sum_{f\delta\sigma} \hat{n}_{f+\delta,\sigma}^p$$
$$+ \frac{U_p}{2} \sum_{f\delta} \hat{n}_{f+\delta,\uparrow}^p \hat{n}_{f+\delta,\downarrow}^p + V_{pd} \sum_{f\delta\sigma\sigma'} \hat{n}_{f\sigma}^d \hat{n}_{f+\delta,\sigma'}^p,$$
$$\hat{T}_{pd} = \sum_{f\delta\sigma} t_{pd}(\delta)(d_{f\sigma}^\dagger p_{f+\delta,\sigma} + h.c.),$$
$$\hat{T}_{pp} = \frac{1}{2} \sum_{f\delta\sigma} t_{pp}(\Delta) p_{f+\delta,\sigma}^\dagger p_{f+\delta+\Delta,\sigma}.$$

Here $d_{f\sigma}^\dagger (d_{f\sigma})$ and $p_{f+\delta,\sigma}^\dagger (p_{f+\delta,\sigma})$ create (annihilate) d and p electrons on copper site f and oxygen site $f + \delta$ with spin projection $\sigma = +1/2, -1/2$, respectively. The Hamiltonian is written in the electronic representation. In

accordance with this we will take into account only the highest (with respect to the energy) orbitals for copper and oxygen ions. The other four p electrons are situated on the deeper orbitals and belong to the ion core. Similarly the eight internal d electrons also belong to the copper ion core and do not participate in the formation of the energy structure in the vicinity of a chemical potential. Further, in the equations δ denotes one of four vectors connecting a copper ion with the oxygen ions in CuO$_2$ plane, Δ is a vector connecting the oxygen ions; $\hat{n}_{f\sigma}^d (\hat{n}_{f+\delta,\sigma}^p)$ is an operator of the $d(p)$ electrons number; ε_d and ε_p are the Cu and O energy levels; U_d, U_p and V_{pd} are intra- and interatomic Coulomb repulsion on Cu sites, O sites and between both sites, respectively; $t_{pd}(\delta)$ and $t_{pp}(\Delta)$ are electron-hopping integrals for hops from copper to oxygen ions and from oxygen to the nearest and next nearest oxygen ions, respectively. Signs of the hopping integrals are chosen so that $t_{pd}(f \pm x/2) = \mp t_{pd}$ and $t_{pd}(f \pm y/2) = \pm t_{pd}$.

The Emery Hamiltonian is typical of the multiband theory of metals in the tight binding representation. The Hamiltonian is of a Hubbard type as it describes both the intra-ionic Coulomb correlations and the processes of hopping between the single-ion states in the Wannier representation.

As is known, the strong intra-atomic correlations are described simplest using the atomic representation. For this description the Hubbard operators [21] built on the basis of one-site (one-cell) states are used [22]. These states are determined as eigenstates of the one-site Hamiltonian which includes all the strong one-site interactions. For further consideration it is convenient to rewrite the Emery Hamiltonian (1) in the atomic representation:

$$\hat{H} = \hat{H}_0 + \hat{T}_{pd} + \hat{T}_{pp}, \tag{2}$$
$$\hat{H}_0 = \sum_f \left(\varepsilon_d^0 \sum_\sigma Z_f^{\sigma\sigma} + (2\varepsilon_d^0 + U_d) Z_f^{22} \right)$$
$$+ \frac{1}{2} \sum_{f\delta} \left(\varepsilon_p^0 \sum_\sigma X_{f+\delta}^{\sigma\sigma} + (2\varepsilon_p^0 + U_p) X_{f+\delta}^{22} \right)$$
$$+ V_{pd} \sum_{f\delta} \left(\sum_\sigma Z_f^{\sigma\sigma} + 2Z_f^{22} \right) \left(\sum_{\sigma'} X_{f+\delta}^{\sigma'\sigma'} + 2X_{f+\delta}^{22} \right),$$
$$\hat{T}_{pd} = \sum_{f\delta\sigma} t_{pd}(\delta) \left\{ \left(Z_f^{\sigma 0} X_{f+\delta}^{0\sigma} + Z_f^{2\bar{\sigma}} X_{f+\delta}^{\bar{\sigma}2} \right. \right.$$
$$\left. \left. + \eta(\sigma) \left(Z_f^{\sigma 0} X_{f+\delta}^{\bar{\sigma}2} + Z_f^{2\bar{\sigma}} X_{f+\delta}^{0\sigma} \right) \right) + h.c. \right\},$$
$$\hat{T}_{pp} = \frac{1}{2} \sum_{f\delta\Delta\sigma} t_{pp}(\Delta) \left(X_{f+\delta}^{\sigma 0} X_{f+\delta+\Delta}^{0\sigma} + X_{f+\delta}^{2\bar{\sigma}} X_{f+\delta+\Delta}^{\bar{\sigma}2} \right.$$
$$\left. + \eta(\sigma) \left(X_{f+\delta}^{\sigma 0} X_{f+\delta+\Delta}^{\bar{\sigma}2} + X_{f+\delta}^{2\bar{\sigma}} X_{f+\delta+\Delta}^{0\sigma} \right) \right),$$

where $Z_f^{mn} = |fm\rangle\langle fn|$ and $X_{f+\delta}^{mn} = |f+\delta, m\rangle\langle f+\delta, n|$ are the Hubbard operators describing the transitions between the one-ion states for copper and oxygen ions; $\eta(\sigma) = \pm 1$ at $\sigma = \pm 1/2$, respectively.

As was mentioned above, without doping the materials under study are insulators despite the electronic d shell

of copper ions is incomplete. Since the p shell of oxygen ions in $La_{2-x}Sr_xCuO_4$ at $x = 0$ is complete and upon weak doping ($x < 0.3$) only a small part of oxygen ions undergo a transition to the $2p^5$ state, during the formation of actual electronic states of the Hilbert space of the oxygen subsystem one can limit the consideration to the states corresponding to the upper Hubbard subband. On each oxygen ion the presence of the strong Coulomb repulsion between two electrons in the upper p states with the opposite projections of the spin moment is assumed. In addition, during the description of the electronic states of copper ions it is reasonable to use the concept of the atomic representation. In the regime of the strong one-site Coulomb repulsion between two electrons on copper ions ($U_d \rightarrow \infty$), only the lower Hubbard subband of the copper d states will contribute to the Fermi excitation dynamics. Reasoning from above and considering the conditions of completeness of the diagonal Hubbard operators of the copper and oxygen ion subsystems

$$Z_f^{00} + Z_f^{\uparrow\uparrow} + Z_f^{\downarrow\downarrow} = 1, \qquad (3)$$

$$X_l^{00} + X_l^{\uparrow\uparrow} + X_l^{\downarrow\downarrow} + X_l^{22} = 1 \qquad (4)$$

and also taking into account that $\langle X_l^{00} \rangle = 0$ upon weak doping, we can rewrite the Emery Hamiltonian as follows:

$$\begin{aligned}
\hat{H} = {} & E_0 + \sum_{f\sigma} \left(\varepsilon_d^0 + 8V_{pd} - 4V_{pd}h_p \right) Z_f^{\sigma\sigma} \\
& + \frac{1}{2} \sum_{f\delta} \left(\left(\varepsilon_p^0 - 2V_{pd} + 2V_{pd}h_d \right) \hat{h}_{f+\delta} \right. \\
& \left. + (2\varepsilon_p^0 + U_p) X_{f+\delta}^{22} \right) \\
& + \sum_{f\delta\sigma} t_{pd}(\delta)\eta(\sigma) \left(Z_f^{\sigma 0} X_{f+\delta}^{\bar{\sigma}2} + X_{f+\delta}^{2\bar{\sigma}} Z_f^{0\sigma} \right) \\
& + \frac{1}{2} \sum_{f\delta\Delta\sigma} t_{pp}(\Delta) X_{f+\delta}^{2\bar{\sigma}} X_{f+\delta+\Delta}^{\bar{\sigma}2} \\
& + V_{pd} \sum_{f\delta} \left(Z_f^{00} - h_d \right) \left(\hat{h}_{f+\delta} - h_p \right), \qquad (5)
\end{aligned}$$

where $\hat{h}_{f+\delta} = X_{f+\delta}^{\uparrow\uparrow} + X_{f+\delta}^{\downarrow\downarrow}$ is the operator of the oxygen holes number and

$$h_d = \frac{1}{N} \sum_f \langle Z_f^{00} \rangle, \quad h_p = \frac{1}{N} \sum_f \langle \hat{h}_{f+\delta} \rangle$$

are the average copper and oxygen holes numbers, respectively.

Since upon doping the holes appear on oxygen ions, between the seed parameters of the model the condition $\varepsilon_p^0 - \varepsilon_d^0 + U_p - 6V_{pd} > 0$ should be met.

Let us now consider some features of form (5) of the Emery Hamiltonian. One can see that the one-site energies of electrons on copper and oxygen ions renormalized by the mean-field effects became dependent of the states of oxygen and copper ions, respectively. This well-known effect was used previously, in particular, in the Falicov-Kimball model [23] for investigation of the transitions with the valency change. An energy shift depends on

the intensity of the intersite Coulomb interaction. Without doping ($h_d = 0$, $h_p = 0$) the renormalized energy of the electron located on a copper ion is $\varepsilon_d = \varepsilon_d^0 + 8V_{pd}$. The term $8V_{pd}$ has simple physical meaning: in the nominal state of the system each electron on a copper ion interacts with eight electrons on the adjacent oxygen ions. Similarly, without doping each electron on an oxygen ion experiences the Hubbard repulsion from the other electron on the same site with the opposite spin projection and interacts with electrons on the two adjacent copper ions. Upon doping the one-site energies of d and p electrons decrease as the average number of holes on the adjacent oxygen and copper ions increase. This leads to a decrease in energy of the Coulomb repulsion as compared to the nominal energy.

The main reason for isolation of the obvious mean-field effects is the need for presentation of the intersite interaction in the form which explicitly reflects the correlation effects. After some simple identical transformations the last Hamiltonian term describing the intersite correlations is written in the desired form. One can see that this term will contribute to the energy structure only in the presence of noticeable fluctuations of the occupation numbers of copper and oxygen ions. The energy $E_0 = 4NV_{pd}h_p(1 - h_d)$ originates, as usual, from isolation of the mean-field effects.

We would like to note that within this approach the insulating state of the system is obtained in a natural way as it is the exact solution of the Schrödinger equation in the absence of doping, i.e. when the sum of holes in the copper and oxygen subsystems is zero.

3 Energy structure

3.1 On consideration of the strong correlations

The method of the consideration of the intersite correlations developed here is natural generalization of the Hubbard's concept of description of the strong one-site correlations [3]. Below we recall the essence of this concept.

Let us consider the Hubbard Hamiltonian

$$\hat{H} = \varepsilon \sum_{f\sigma} \hat{n}_{f\sigma} + \sum_{fm\sigma} t_{fm} a_{f\sigma}^\dagger a_{m\sigma} + \frac{U}{2} \sum_{f\sigma} \hat{n}_{f\sigma} \hat{n}_{f\bar{\sigma}}, \quad (6)$$

and write the first exact equation of motion for the two-time retarded anticommutator Green's function:

$$\begin{aligned}
(\omega - \varepsilon)\langle\langle a_{f\sigma} | a_{g\sigma}^\dagger \rangle\rangle_\omega = {} & \delta_{fg} + \sum_m t_{fm} \langle\langle a_{m\sigma} | a_{g\sigma}^\dagger \rangle\rangle_\omega \\
& + U \langle\langle a_{f\sigma} \hat{n}_{f\bar{\sigma}} | a_{g\sigma}^\dagger \rangle\rangle_\omega. \qquad (7)
\end{aligned}$$

It is seen that equation (7) contains the Green's function of higher order by the second quantized operators. It is important that the function is preceded by energy factor U reflecting the Coulomb interaction between two electrons with the opposite spin projections located on one site. Under the condition of the strong correlations, factor U is

the main energy parameter; therefore, in the operators describing the one-site processes decoupling cannot be used. It means that the corresponding high Green's function needs in its own equation of motion:

$$(\omega - \varepsilon - U)\langle\langle a_{f\sigma}\hat{n}_{f\bar{\sigma}}|a_{g\sigma}^{\dagger}\rangle\rangle_{\omega} = \delta_{fg}\langle\hat{n}_{f\bar{\sigma}}\rangle$$
$$+ \sum_{m} t_{fm}\Bigg\{\langle\langle a_{m\sigma}\hat{n}_{f\bar{\sigma}}|a_{g\sigma}^{\dagger}\rangle\rangle_{\omega} + \langle\langle a_{f\sigma}a_{f\bar{\sigma}}^{\dagger}a_{m\bar{\sigma}}|a_{g\sigma}^{\dagger}\rangle\rangle_{\omega}$$
$$- \langle\langle a_{f\sigma}a_{m\bar{\sigma}}^{\dagger}a_{f\bar{\sigma}}|a_{g\sigma}^{\dagger}\rangle\rangle_{\omega}\Bigg\}. \quad (8)$$

This equation also contains the high-order Green's functions, but with small energy factor t_{fm}. In these functions decoupling is implemented only relative to the multisite operators. It allows to describe correctly the one-site correlations and characteristics of the Mott-Hubbard insulator.

As is known the solution of the system of equations (7)–(8) in the quasi-momentum representation yields an energy spectrum consisting of two Hubbard subbands. The lower band corresponds to the motion of an electron over the sites when other electrons on these sites are absent. The upper band is formed due to hopping over the sites where electrons with opposite spin projections are already located. Therefore, the energy of such a band includes the shift by a value of Coulomb repulsion U.

Having generalized the Hubbard's concept for consideration of the strong one-site correlations to the intersite correlations we come to the conclusion that the high-order Green's functions which appear in the system of equations of motion with intersite Coulomb interaction parameter V_{pd} should not be reduced to simpler functions. Consequently, these functions need in the corresponding equations of motion which would make exact allowance for all the contributions of the intersite correlations. Only the terms containing no large energy factors can be simplified.

For the correct description of the intersite correlations it appears the most effective to introduce an orthogonal set of the irreducible operators with the subsequent use of the Zwanzig-Mori projection technique [24,25] in other to close the equations of motion for the extended set of the Green's function.

3.2 Orthogonal basis of the irreducible operators

We introduce the orthogonal set of the basis operators

$$\left\{Z_f^{0\sigma}, \; X_{f+\delta^+}^{\bar{\sigma}2}, \; \hat{\Phi}_f^{\sigma}, \; \hat{\Psi}_{f+\delta^+}^{\sigma}\right\}, \quad (9)$$

where two last basis elements are determined as

$$\hat{\Phi}_f^{\sigma} = \sum_{\delta} Z_f^{0\sigma}\left(\hat{h}_{f+\delta} - h_p\right),$$
$$\hat{\Psi}_{f+\delta^+}^{\sigma} = X_{f+\delta^+}^{\bar{\sigma}2}\left(Z_f^{00} + Z_{f+2\delta^+}^{00} - 2h_d\right). \quad (10)$$

In this case the concept of orthogonality is based on the following definition of the scalar product of two quasi-Fermi operators:

$$(\hat{A}, \hat{B}) = \langle\{\hat{A}, \hat{B}\}_+\rangle = \langle\hat{A}\hat{B} + \hat{B}\hat{A}\rangle. \quad (11)$$

In accordance with definition (11) the norms of the basis elements are

$$\langle\{Z_f^{0\sigma}, Z_f^{\sigma0}\}_+\rangle = 1 - \frac{n_d}{2},$$
$$\langle\{X_{f+\delta^+}^{\bar{\sigma}2}, X_{f+\delta^+}^{2\bar{\sigma}}\}_+\rangle = \frac{n_p}{2} = 1 - \frac{h_p}{2},$$
$$\langle\{\hat{\Phi}_f^{\sigma}, (\hat{\Phi}_f^{\sigma})^{\dagger}\}_+\rangle = 4h_p(1-h_p)\left(1 - \frac{n_d}{2}\right),$$
$$\langle\{\hat{\Psi}_{f+\delta^+}^{\sigma}, (\hat{\Psi}_{f+\delta^+}^{\sigma})^{\dagger}\}_+\rangle = 2h_d(1-h_d)\left(1 - \frac{h_p}{2}\right). \quad (12)$$

Let us consider the physical meaning of operators (10). Operator $\hat{\Phi}_f^{\sigma}$ corresponds to the electron annihilation on copper ion f when the intensity of the process depends on the deviation of configurations of the nearest oxygen ions from the average statistical configuration. Similarly, operator $\hat{\Psi}_{f+\delta^+}^{\sigma}$ reflects the electron annihilation on oxygen ion $f + \delta^+$ with transferring this ion from the double occupied state to the single-electron state. The intensity of this process depends on the deviation of the electronic configurations of the two copper ions nearest to site $f+\delta^+$ from the average statistical configuration.

The site indices are recorded using the vectors $\delta^+ \in \left\{\left(\frac{a}{2},0\right), \left(0,\frac{a}{2}\right)\right\}$ which relate a copper ion to merely two of the four nearest oxygen ions. This limitation is obvious as, otherwise, the introduced basis would make allowance for operators $\hat{\Psi}_{f+\delta^+}^{\sigma}$ twice.

Basis (9) does not contain the operators describing more than one hole on oxygen ions in the nearest neighborhood of a copper ion. This simplification is justified, because upon weak doping the condition $h_p \ll 1$ should be met. Indeed, under the conditions when the number of copper holes per unit cell of CuO_2 plane $h_d \simeq 1$ and the number of oxygen holes per unit cell $h_p \ll 1$, the interaction between oxygen holes can be disregarded. Actually, the specific energy of this interaction $\sim V_{pp}h_p^2$ is quadratic in the small parameter h_p. At the same time, due to condition $h_d \simeq 1$, the interaction between the holes on Cu and O ions $\sim V_{pd}h_ph_d \simeq V_{pd}h_p$ becomes important, because it is linear in h_p. Thus, the problem of the energy structure of the Emery model in the case of weak doping involves the gas parameter $h_p \ll 1$. The number of the equations of motion is significantly reduced due to the use of the gas approximation.

3.3 The equations of motion and self-consistency equations

The exact equation of motion in the Heisenberg representation is

$$i\frac{d}{dt}Z_f^{0\sigma} = (\varepsilon_d - 4V_{pd}h_p)Z_f^{0\sigma} - V_{pd}\hat{\Phi}_f^{\sigma}$$
$$+ \sum_{\delta} t_{pd}(\delta)\eta(\sigma)\Big((Z_f^{00} + Z_f^{\sigma\sigma})X_{f+\delta}^{\bar{\sigma}2} - Z_f^{\bar{\sigma}\sigma}X_{f+\delta}^{\sigma2}\Big). \quad (13)$$

It is seen that the intersite correlations lead to trapping more complicated operator $\hat{\Phi}_f^{\sigma}$ which describes a correlated process of the electron annihilation on a copper ion.

This correlation is related to the possibility of changing valency of the nearest oxygen ions. The obtained equation of motion evidences expediency of isolation of the mean-field effects implemented in Section 2 via the intersite interactions.

The second exact equation of motion takes the form

$$
i\frac{d}{dt}\left(X_{f+\delta^+}^{\bar\sigma 2}\right) = (\varepsilon_p - 2V_{pd}h_d)X_{f+\delta^+}^{\bar\sigma 2} - V_{pd}\eta(\sigma)\hat\Psi_{f+\delta^+}^{\sigma}
$$
$$
+t_{pd}(\delta^+)\,\eta(\sigma)\Big(\big(X_{f+\delta^+}^{\bar\sigma\bar\sigma} + X_{f+\delta^+}^{22}\big)\big(Z_f^{0\sigma} - Z_{f+2\delta^+}^{0\sigma}\big)
$$
$$
-X_{f+\delta^+}^{\bar\sigma\sigma}\big(Z_f^{0\bar\sigma} - Z_{f+2\delta^+}^{0\bar\sigma}\big)\Big)
$$
$$
+\sum_{\Delta} t_{pp}(\Delta)\Big(\big(X_{f+\delta^+}^{\bar\sigma\bar\sigma} + X_{f+\delta^+}^{22}\big)X_{f+\delta^++\Delta}^{\bar\sigma 2}
$$
$$
+X_{f+\delta^+}^{\bar\sigma\sigma}X_{f+\delta^++\Delta}^{\sigma 2}\Big). \tag{14}
$$

Again, as in equation (13), the intersite correlations lead to trapping irreducible operator $\hat\Psi_{f+\delta^+}^{\sigma}$. Two remaining equations for the basis operators are

$$
i\frac{d}{dt}\hat\Phi_f^{\sigma} = (\varepsilon_d - 4V_{pd}h_p)\hat\Phi_f^{\sigma} + \sum_{\delta\delta_1} t_{pd}(\delta_1)\eta(\sigma)
$$
$$
\times\Big(\big(Z_f^{00} + Z_f^{\sigma\sigma}\big)X_{f+\delta_1}^{\bar\sigma 2} - Z_f^{\bar\sigma\sigma}X_{f+\delta_1}^{\sigma 2}\Big)\big(\hat h_{f+\delta} - h_p\big)
$$
$$
+\sum_{\delta} t_{pd}(\delta)\eta(\sigma)Z_f^{00}X_{f+\delta}^{\bar\sigma 2}
$$
$$
-\sum_{\delta\sigma_1} t_{pd}(\delta)\eta(\sigma_1)Z_f^{0\sigma}\Big(Z_{f+2\delta}^{\sigma_1 0}X_{f+\delta}^{\bar\sigma_1 2} - X_{f+\delta}^{2\bar\sigma_1}Z_{f+2\delta}^{0\sigma_1}\Big)
$$
$$
+\sum_{\delta\Delta\sigma_1} t_{pp}(\Delta)Z_f^{0\sigma}\Big(X_{f+\delta+\Delta}^{2\bar\sigma_1}X_{f+\delta}^{\bar\sigma_1 2} - X_{f+\delta}^{2\bar\sigma_1}X_{f+\delta+\Delta}^{\bar\sigma_1 2}\Big)
$$
$$
-V_{pd}\sum_{\delta\delta_1} Z_f^{0\sigma}\big(\hat h_{f+\delta_1} - h_p\big)\big(\hat h_{f+\delta} - h_p\big), \tag{15}
$$

and

$$
i\frac{d}{dt}\hat\Psi_{f+\delta^+}^{\sigma} = (\varepsilon_p - 2V_{pd}h_d)\hat\Psi_{f+\delta^+}^{\sigma} + t_{pd}(\delta^+)
$$
$$
\times\Big(\big(X_{f+\delta^+}^{\bar\sigma\bar\sigma} + X_{f+\delta^+}^{22}\big)\big(Z_f^{0\sigma} - Z_{f+2\delta^+}^{0\sigma}\big)
$$
$$
-X_{f+\delta^+}^{\bar\sigma\sigma}\big(Z_f^{0\bar\sigma} - Z_{f+2\delta^+}^{0\bar\sigma}\big)\Big)\big(Z_f^{00} + Z_{f+2\delta^+}^{00} - 2h_d\big)
$$
$$
+\sum_{\Delta} t_{pp}(\Delta)\eta(\sigma)\Big(\big(X_{f+\delta^+}^{\bar\sigma\bar\sigma} + X_{f+\delta^+}^{22}\big)X_{f+\delta^++\Delta}^{\bar\sigma 2}
$$
$$
+X_{f+\delta^+}^{\bar\sigma\sigma}X_{f+\delta^++\Delta}^{\sigma 2}\Big)\big(Z_f^{00} + Z_{f+2\delta^+}^{00} - 2h_d\big)
$$
$$
-V_{pd}\eta(\sigma)X_{f+\delta^+}^{\bar\sigma 2}\big(Z_f^{00} + Z_{f+2\delta^+}^{00} - 2h_d\big)
$$
$$
\times\big(Z_f^{00} + Z_{f+2\delta^+}^{00} - 2h_d\big)
$$
$$
+\sum_{\sigma_1} t_{pd}(\delta^+)\eta(\sigma)\eta(\sigma_1)X_{f+\delta^+}^{\bar\sigma\bar\sigma_1}\big(Z_f^{0\sigma_1} - Z_{f+2\delta^+}^{0\sigma_1}\big)
$$
$$
+\sum_{\delta(\delta\neq\delta^+)}\sum_{\sigma_1} t_{pd}(\delta)\eta(\sigma)\eta(\sigma_1)\Big(X_{f+\delta^+}^{\bar\sigma 2}X_{f+\delta}^{2\bar\sigma_1}Z_f^{0\sigma_1}
$$
$$
-X_{f+\delta^+}^{\bar\sigma 2}Z_f^{\sigma_1 0}X_{f+\delta}^{\bar\sigma_1 2}\Big). \tag{16}
$$

In equations (13)–(16) the notations $\varepsilon_d = \varepsilon_d^0 + 8V_{pd}$ and $\varepsilon_p = \varepsilon_p^0 + U_p + 2V_{pd}$ for the one-site energies of electrons on copper and oxygen ions renormalized by the intersite correlations are used. Note that ε_d and ε_p should be considered as fitting parameters for comparison of the experimental and theoretical data.

For closing the system of equations (13)–(16) we use the Zwanzig-Mori projection technique [24,25], i.e. each term of the right parts of the equations are projected onto a subspace which represents a linear shell formed by basis operators (9). The algorithm of projection of arbitrary operator $\hat A$ onto basis vector e consists in calculation of the scalar product $(\hat A, e)$ and multiplication of the obtained value by $e/(e,e)$. For the basis introduced above the aforesaid means that the procedure of decomposition of arbitrary operator $\hat A$ is reduced to the calculation of the projection component as follows:

$$
\hat A \to \sum_g \Bigg(\frac{\langle\{\hat A, Z_g^{\sigma 0}\}_+\rangle}{\langle\{Z_g^{0\sigma}, Z_g^{\sigma 0}\}_+\rangle}Z_g^{0\sigma} + \frac{\langle\{\hat A, X_g^{2\bar\sigma}\}_+\rangle}{\langle\{X_g^{\bar\sigma 2}, X_g^{2\bar\sigma}\}_+\rangle}X_g^{\bar\sigma 2}
$$
$$
+\frac{\langle\{\hat A, (\hat\Phi_g^\sigma)^\dagger\}_+\rangle}{\langle\{\hat\Phi_g^\sigma, (\hat\Phi_g^\sigma)^\dagger\}_+\rangle}\hat\Phi_g^\sigma + \frac{\langle\{\hat A, (\hat\Psi_g^\sigma)^\dagger\}_+\rangle}{\langle\{\hat\Psi_g^\sigma, (\hat\Psi_g^\sigma)^\dagger\}_+\rangle}\hat\Psi_g^\sigma\Bigg). \tag{17}
$$

The linear approximation tolerates ignoring the kinetic correlators appearing after projection and limiting the consideration to spatially homogeneous solutions. Applying Fourier transformations to the Green's functions

$$
\langle\langle Z_f^{0\sigma}|Z_{f'}^{\sigma 0}\rangle\rangle_\omega = \frac{1}{N}\sum_{\boldsymbol k} e^{i\boldsymbol k(\boldsymbol R_f - \boldsymbol R_{f'})}\langle\langle Z_{\boldsymbol k\sigma}|Z_{\boldsymbol k\sigma}^\dagger\rangle\rangle,
$$
$$
\langle\langle\eta(\sigma)X_{f+x/2}^{\bar\sigma 2}|Z_{f'}^{\sigma 0}\rangle\rangle_\omega =
$$
$$
\frac{1}{N}\sum_{\boldsymbol k} e^{i\boldsymbol k(\boldsymbol R_f + \boldsymbol R_{x/2} - \boldsymbol R_{f'})}\langle\langle X_{\boldsymbol k\sigma}|Z_{\boldsymbol k\sigma}^\dagger\rangle\rangle,
$$
$$
\langle\langle\eta(\sigma)Y_{f+y/2}^{\bar\sigma 2}|Z_{f'}^{\sigma 0}\rangle\rangle_\omega =
$$
$$
\frac{1}{N}\sum_{\boldsymbol k} e^{i\boldsymbol k(\boldsymbol R_f + \boldsymbol R_{y/2} - \boldsymbol R_{f'})}\langle\langle Y_{\boldsymbol k\sigma}|Z_{\boldsymbol k\sigma}^\dagger\rangle\rangle,
$$
$$
\langle\langle\Phi_f^\sigma|Z_{f'}^{\sigma 0}\rangle\rangle_\omega = \frac{1}{N}\sum_{\boldsymbol k} e^{i\boldsymbol k(\boldsymbol R_f - \boldsymbol R_{f'})}\langle\langle\Phi_{\boldsymbol k\sigma}|Z_{\boldsymbol k\sigma}^\dagger\rangle\rangle,
$$
$$
\langle\langle\Psi_{f+x/2}^\sigma|Z_{f'}^{\sigma 0}\rangle\rangle_\omega = \frac{1}{N}\sum_{\boldsymbol k} e^{i\boldsymbol k(\boldsymbol R_f + \boldsymbol R_{x/2} - \boldsymbol R_{f'})}\langle\langle\Psi_{\boldsymbol k\sigma}^x|Z_{\boldsymbol k\sigma}^\dagger\rangle\rangle,
$$
$$
\langle\langle\Psi_{f+y/2}^\sigma|Z_{f'}^{\sigma 0}\rangle\rangle_\omega = \frac{1}{N}\sum_{\boldsymbol k} e^{i\boldsymbol k(\boldsymbol R_f + \boldsymbol R_{y/2} - \boldsymbol R_{f'})}\langle\langle\Psi_{\boldsymbol k\sigma}^y|Z_{\boldsymbol k\sigma}^\dagger\rangle\rangle, \tag{18}
$$

we obtain the closed system of equations in the quasi-momentum representation:

$$
(\omega - \varepsilon_d + 4V_{pd}h_p)\langle\langle Z_{\boldsymbol k\sigma}|Z_{\boldsymbol k\sigma}^\dagger\rangle\rangle = N_d
$$
$$
-iN_d\Big(S_x\langle\langle X_{\boldsymbol k\sigma}|Z_{\boldsymbol k\sigma}^\dagger\rangle\rangle - S_y\langle\langle Y_{\boldsymbol k\sigma}|Z_{\boldsymbol k\sigma}^\dagger\rangle\rangle\Big)
$$
$$
-\frac{i}{4}\Big(S_x\langle\langle\Psi_{\boldsymbol k\sigma}^x|Z_{\boldsymbol k\sigma}^\dagger\rangle\rangle - S_y\langle\langle\Psi_{\boldsymbol k\sigma}^y|Z_{\boldsymbol k\sigma}^\dagger\rangle\rangle\Big)
$$
$$
-V_{pd}\langle\langle\Phi_{\boldsymbol k\sigma}|Z_{\boldsymbol k\sigma}^\dagger\rangle\rangle, \tag{19}
$$

$$\left(\omega - \varepsilon_p + 2V_{pd}h_d - \frac{n_p}{2}C_y\right)\langle\langle X_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle =$$
$$i\frac{n_p}{2}S_x\langle\langle Z_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle + \frac{n_p}{2}V_{xy}\langle\langle Y_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle$$
$$-\frac{i}{8}S_x\langle\langle \Phi_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle - V_{pd}\langle\langle \Psi^x_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle, \quad (20)$$

$$\left(\omega - \varepsilon_p + 2V_{pd}h_d - \frac{n_p}{2}C_x\right)\langle\langle Y_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle =$$
$$-i\frac{n_p}{2}S_y\langle\langle Z_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle + \frac{n_p}{2}V_{xy}\langle\langle X_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle$$
$$+\frac{i}{8}S_y\langle\langle \Phi_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle - V_{pd}\langle\langle \Psi^y_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle, \quad (21)$$

$$\left(\omega - \varepsilon_d + 4V_{pd}h_p + V_{pd}(1 - 2h_p)\right)\langle\langle \Phi_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle =$$
$$i(N_dh_p - h_d)\Big(S_x\langle\langle X_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle - S_y\langle\langle Y_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle\Big)$$
$$+i\left(\frac{h_p}{4} - \frac{1}{2}\right)\Big(S_x\langle\langle \Psi^x_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle - S_y\langle\langle \Psi^y_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle\Big)$$
$$-4V_{pd}h_p(1 - h_p)\langle\langle Z_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle, \quad (22)$$

$$\left(\omega - \varepsilon_p + 2V_{pd}h_d - \frac{n_p}{2}C_y + V_{pd}(1 - 2h_d)\right)$$
$$\times \langle\langle \Psi^x_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle = -i\left(\frac{n_p}{2}h_d - \frac{h_p}{2}\right)S_x\langle\langle Z_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle$$
$$-2V_{pd}h_d(1 - h_d)\langle\langle X_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle$$
$$+i\left(\frac{h_d}{4} + \frac{1}{8}\right)S_x\langle\langle \Phi_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle + \frac{n_p}{2}V_{xy}\langle\langle \Psi^y_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle, \quad (23)$$

$$\left(\omega - \varepsilon_p + 2V_{pd}h_d - \frac{n_p}{2}C_x + V_{pd}(1 - 2h_d)\right)$$
$$\times \langle\langle \Psi^y_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle = i\left(\frac{n_p}{2}h_d - \frac{h_p}{2}\right)S_y\langle\langle Z_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle$$
$$-2V_{pd}h_d(1 - h_d)\langle\langle Y_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle$$
$$-i\left(\frac{h_d}{4} + \frac{1}{8}\right)S_y\langle\langle \Phi_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle + \frac{n_p}{2}V_{xy}\langle\langle \Psi^x_{\boldsymbol{k}\sigma}|Z^\dagger_{\boldsymbol{k}\sigma}\rangle\rangle. \quad (24)$$

Here the following notations are used:

$$S_x = 2t_{pd}\sin\left(\frac{k_xa}{2}\right), \; S_y = 2t_{pd}\sin\left(\frac{k_ya}{2}\right),$$
$$V_{xy} = 4t_{pp}\sin\left(\frac{k_xa}{2}\right)\sin\left(\frac{k_ya}{2}\right), \; N_d = 1 - \frac{n_d}{2},$$
$$C_y = -2t'_{pp1}\cos(k_xa) + 2t'_{pp}\cos(k_ya)$$
$$+4t''_{pp}\cos(k_xa)\cos(k_ya) + 2t'''_{pp}\cos(2k_ya),$$
$$C_x = -2t'_{pp1}\cos(k_ya) + 2t'_{pp}\cos(k_xa)$$
$$+4t''_{pp}\cos(k_xa)\cos(k_ya) + 2t'''_{pp}\cos(2k_xa). \quad (25)$$

Using the spectral theorem [26], it is easy to write the system of self-consistency equations for obtaining the dependence of the energy structure on doping:

$$\frac{n_d}{2} = \frac{1}{N}\sum_{\boldsymbol{k}}\sum_{i=1}^{6}A_i(E_{i\boldsymbol{k}})f(E_{i\boldsymbol{k}}),$$
$$n_2^p = \frac{1}{N}\sum_{\boldsymbol{k}}\sum_{i=1}^{6}B_i(E_{i\boldsymbol{k}})f(E_{i\boldsymbol{k}}),$$
$$n_p = n_2^p + 1,$$
$$n_d + 2n_p = 5 - P, \quad (26)$$

where $f(x) = (\exp(\frac{x-\mu}{T}) + 1)^{-1}$ is the Fermi-Dirac function, n_2^p is the concentration of the double occupied oxygen states, and P is the doping parameter. The spectral intensities are

$$A_i(E_{i\boldsymbol{k}}) = \sum_i \frac{\Delta_Z(E_{i\boldsymbol{k}})}{\prod_{j\neq i}(E_{i\boldsymbol{k}} - E_{j\boldsymbol{k}})},$$
$$B_i(E_{i\boldsymbol{k}}) = \sum_i \frac{\Delta_X(E_{i\boldsymbol{k}})}{\prod_{j\neq i}(E_{i\boldsymbol{k}} - E_{j\boldsymbol{k}})}. \quad (27)$$

Here the notations are used:

$$\Delta_Z(E_{i\boldsymbol{k}}) = N_dM_{11}(E_{i\boldsymbol{k}}), \; \Delta_X(E_{i\boldsymbol{k}}) = \frac{n_p}{2}M_{22}(E_{i\boldsymbol{k}}), \quad (28)$$

where M_{ij} is the subdeterminant obtained from the main matrix of the system of equations (19)–(24) by deletion of the i-th row and the j-th column.

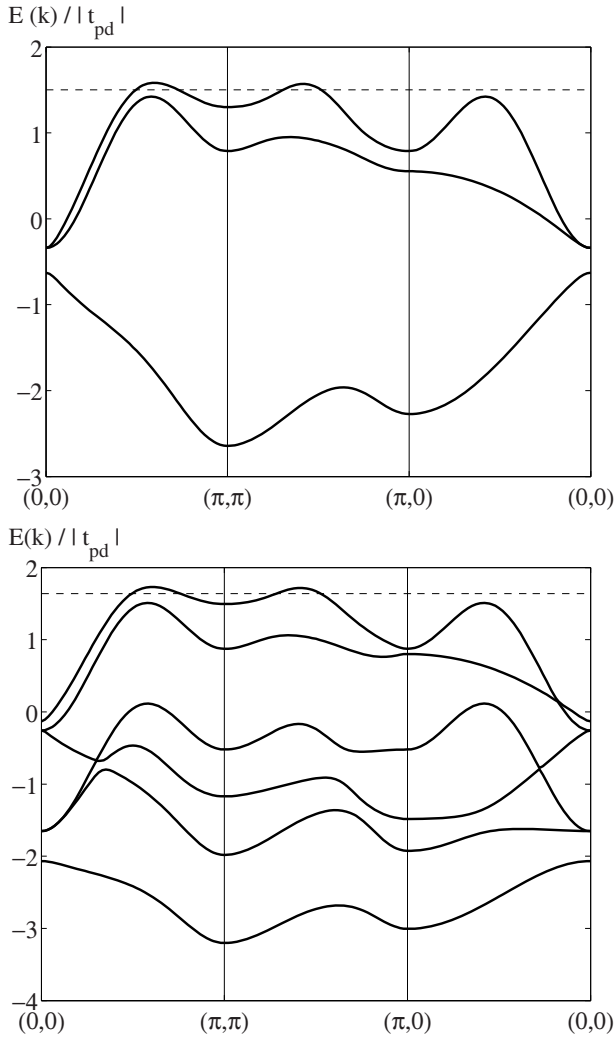### 3.4 Bands of the fluctuation states

It is known that calculation of the energy structure of the Emery model in the Hartree-Fock approximation yields a three-band picture (Fig. 2, on top). The calculation is made for the set of parameters close to commonly used (in terms of $|t_{pd}|$):

$$\varepsilon_d^0 = -10.4, \quad \varepsilon_p^0 = -7.1, \quad t_{pp} = 0.2, \quad t'_{pp} = -0.3,$$
$$t'_{pp1} = -0.2, \quad t''_{pp} = 0.01, \quad t'''_{pp} = -0.3,$$
$$U_p = 5, \quad V_{pd} = 1.3. \quad (29)$$

In this case the lower band is formed mainly by the copper d states, while the two upper bands with a maximum in the vicinity of $(\frac{\pi}{2}, \frac{\pi}{2})$ correspond to the hybridized p_x and p_y oxygen states. Without doping the chemical potential is located above the top of the upper band and the system is a Mott-Hubbard insulator. Upon doping holes appear in the system and the chemical potential drops falling in the upper band. Thus, the system becomes metallic.
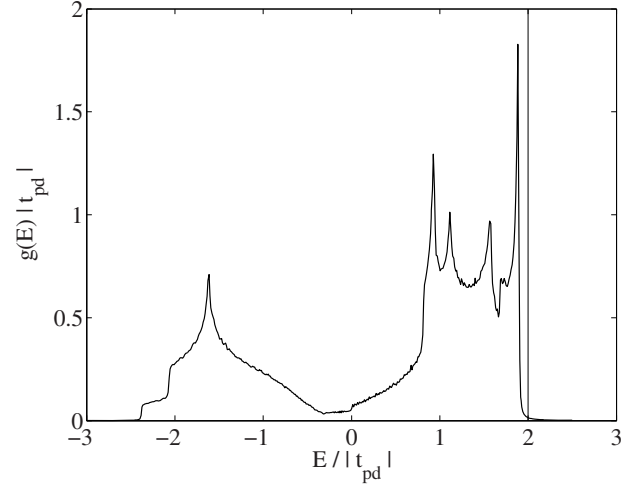
Figure 2 (bottom) depicts the energy spectrum of the model under consideration. The spectrum was obtained by solving the system of equations (19)–(24) at the same parameter values and doping level. The qualitative difference between the band picture obtained and that typical of the Hartree-Fock approximation is that the correct account for the intersite correlations leads to the appearance of additional energy levels in the energy structure of the Emery model.

The physical origin of three additional energy levels is the following. Without our approach in the absence of doping there are two electrons on each oxygen ion. Thus, considering the intersite interaction, excitation energy ε_d of an electron located on a copper ion consists of the seed energy and energy of the interaction with surrounding oxygen electrons, i.e. $\varepsilon_d = \varepsilon_d^0 + 8V_{pd}$. The hopping processes cause splitting of this energy level, so the latter turns into an energy band.

Fig. 2. Band picture of the Emery model in the limit of strong one-site correlations with account for the intersite correlations in the Hartree-Fock approximation (top) and with account for the bands of the fluctuation states (bottom) for the set of parameters (29) at the doping level $P = 0.27$. Dashed lines show the chemical potential.
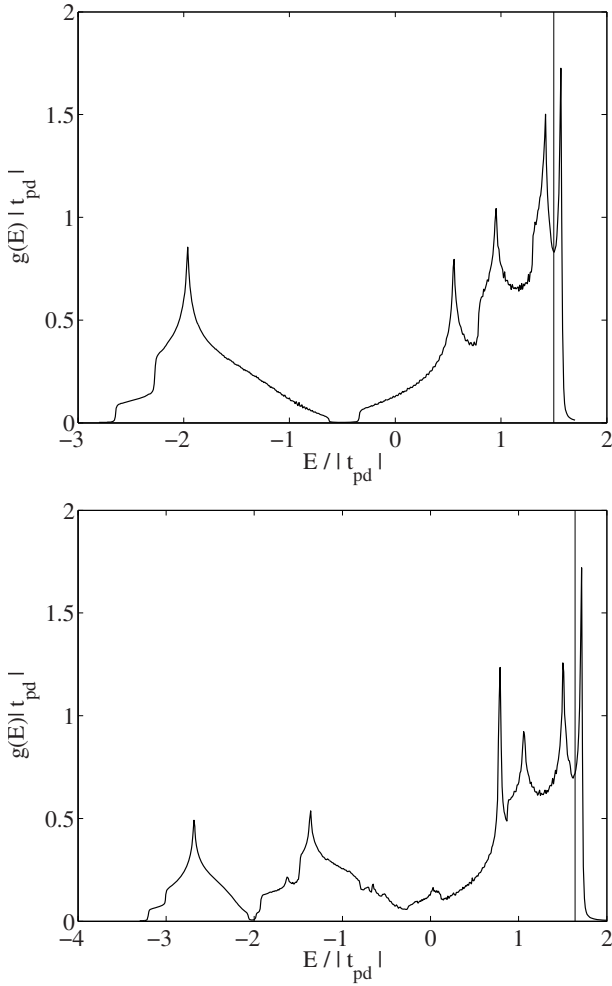
Fig. 3. Density of states of the Emery model in the limit of strong one-site correlations with account for the bands of the fluctuation states without doping for the set of parameters (29). Vertical straight line shows the chemical potential.

rence of three additional energy levels in the energy structure of the Emery model. At a large value of the intersite Coulomb interaction the fluctuation levels are noticeably separated from the initial one-site energy levels.

Here we do not consider the case when each of two copper ion adjacent to oxygen ions loses one electron. This approximation is justified as statistical weight of the considered configurations is relatively small. Otherwise we would have to consider also the fluctuation levels $\tilde{\varepsilon}_p = \varepsilon_p - 2V_{pd}$. The calculations we made to check the validity of this approximation showed that the contribution of the states with the energy $\tilde{\varepsilon}_p = \varepsilon_p - 2V_{pd}$ at the doping levels attainable experimentally is negligible.

Thus, the formation of the additional energy levels is caused by changing energy of the electron located on a site if near this site the electronic configurations deviate from nominal ones. Consequently, the occurrence of the new levels is related to the charge fluctuations. The hopping processes lead to spreading the fluctuation levels into energy bands, which we name the bands of the fluctuation states (BFS).

We would like to emphasize that the occurrence of the BFS in the Emery model due to the intersite correlations is qualitatively similar to the occurrence of two Hubbard subbands at the strong intra-atomic repulsion. Obviously, upon weak doping the spectral intensity of the BFS will be small and their contribution to the integrated energy structure will be insignificant (Fig. 3). It is clear, that in this case the energy structure is similar to that following from the theory which takes into account the intersite correlations in the Hartree-Fock approximation (Fig. 4, top). However, if the concentration of holes in the system increases, then at the doping levels $P = 0.2 \div 0.3$ the picture becomes qualitative different. With an increase in number of holes in the system or in intensity of the hopping processes the spectral intensity of the BFS, determined by the root-mean-square fluctuations of the occupation numbers

If there are holes in the system, then there will be only one, not two, electron on some oxygen ions. In this case the one-site excitation energy of an electron located on the copper ion adjacent to the mentioned oxygen ions will be $\varepsilon_d^0 + 7V_{pd}$ instead of $\varepsilon_d^0 + 8V_{pd}$. Thus, the additional energy levels for d electrons $\tilde{\varepsilon}_d = \varepsilon_d - V_{pd}$ appear in the system; they are fluctuation levels located below initial level ε_d by V_{pd}. Similarly, for the oxygen states the fluctuation levels will also appear as soon as holes get in the system upon doping. Indeed, due to the hybridization processes some copper ions lose one electron. Then the excitation energy of an electron on an oxygen ion will be $\tilde{\varepsilon}_p = \varepsilon_p - V_{pd}$ instead of the nominal value $\varepsilon_p = \varepsilon_p^0 + U_p + 2V_{pd}$. It will lead to the formation of the fluctuation level. As there are two oxygen ions in a unit cell of the CuO_2 plane, two fluctuation levels corresponding to the oxygen orbitals per unit cell will occur. These circumstances determine the occur-

Fig. 4. Density of states of the Emery model in the limit of strong one-site correlations with account for the intersite correlations in the Hartree-Fock approximation (top) and with account for the bands of the fluctuation states (bottom) for the set of parameters (29) at the doping level $P = 0.27$. Vertical straight lines show the chemical potential.

increases and the new bands start playing an important role. As a result, with an increase in doping level the spectral weight is redistributed between the ordinary bands and the BFS in favour of the latter. This induces the occurrence of an additional peak of the density of states of the model determined as

$$g(\omega) = \frac{1}{N} \sum_{\boldsymbol{k}} \sum_{i} \big(A_i(E_{i\boldsymbol{k}}) + B_i(E_{i\boldsymbol{k}}) \big) \delta(\omega - E_{i\boldsymbol{k}}) \quad (30)$$

($\delta(x)$ is the Dirac delta-function), in the vicinity of the fluctuation band of the copper d states, as well as the noticeable increase in the density of states near the oxygen BFS (Fig. 4, at the bottom). The top plot calculated with allowance made for the intersite correlations in the Hartree-Fock approximation shows that at the doping level $P = 0.27$ the chemical potential of the system falls in a dip of the density of states. When the BFS are taken into account, the above-mentioned redistribution of the spectral intensity between the ordinary bands and the BFS

occurs which favors the increase in the dip of the density of states at the Fermi level (Fig. 4, at the bottom).

It must be noted that in the hypothetical limit when there would be one hole strictly on each oxygen ion, the fluctuation levels $\tilde{\varepsilon}_p = \varepsilon_p - V_{pd}$ would turn into the basic ones with the formation of the corresponding band and the spectral intensity of the latter would be the highest.

Let us now consider the physical meaning of the requirement for smallness of electron-hopping integral t_{pd} (narrow band) as compared to the intensity of intersite Coulomb correlations V_{pd}. As was mentioned above, when V_{pd} is significant the energy spread between the ordinary and fluctuation levels becomes large. Under these conditions at relatively small t_{pd} (small kinetic energy) an electron getting on the site in the vicinity of which there are ions with other valency will be in the state with the modified energy for some time (until hopping to another site). For this reason this modified energy will influence the formation of the resulting energy structure.

In the opposite case, when kinetic energy of an electron is large as compared to the energy of the intersite correlations, an electron will continuously move over the lattice sites having no time to follow the change in the one-site energies caused by the formation of the electronic configurations with other valency of the nearest surrounding. Therefore, the fluctuations of the one-site energies will close and the statistically averaged picture of the band states will form.

4 Conclusion

In the framework of the Emery model in the strongly correlated regime without involving the cluster perturbation theory the effect of the intersite Coulomb interaction of fermions on the electronic energy structure of HTSC has been studied. The method for the correct description of the intersite correlations using the extended orthogonal basis of the irreducible operators has been developed. With a use of the Zwanzig-Mori projection technique, the closed system of equations describing the dynamics of the Fermi excitations has been obtained and solved for the extended set of the Green's functions.

The study of the energy structure carried out by the developed method has shown that the inclusion of the intersite correlations effects yields not only quantitative changes but also a number of qualitatively new features. We emphasize that we are speaking of the intersite correlations and not of the intersite interaction. Indeed, the most part of the interaction which is reduced to the mean-field effects is easily described by the above-mentioned renormalization of the one-site energies of the copper and oxygen orbitals, whereas the description of the correlation effects would demand the higher irreducible Green's functions.

The qualitatively new effects found are the following. The first one is the occurrence of new energy bands due to the charge fluctuations. The second effect is redistribution of the spectral intensity between the ordinary bands and fluctuation bands, which is especially important as it

can induce the pseudogap state of a strongly correlated system upon doping. The final answer to the question whether this redistribution of the integrated density of states can induce the spectral intensity modulation on a Fermi contour requires closer examination, which is beyond this study.

To conclude with, we note that the proposed method of the account for the strong intersite Coulomb correlations represents natural generalization of the approach widely used in theory of strongly correlated systems with the one-site correlations. The application of our method shows that the strong intersite correlations induce quantitative changes in the energy structure of the Emery model. It means that the account for the intersite correlations is important for interpretation of the low-energy properties of the HTSC described by the three-band Emery model.

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